Molten Salt Reactor Neutronic and Fuel Cycle Sensitivity and Uncertainty Analysis[1]

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INTRODUCTION

Neutronic and fuel cycle simulations of Molten Salt Reactors (MSRs) must account for the isotopic change of the fuel salt under irradiation, including continuous feeds, removals, and additional chemical behaviors that impact fuel salt composition (e.g., corrosion or plating). Among many time-dependent quantities, these simulations predict reactivity coefficients, fueling rates, fission product generation rates, and waste accumulation rates. Uncertainties in nuclear data and assumed reactor design and operational parameters due to tolerances and instrumentation limitations lend to uncertainties in these predicted time-dependent quantities.

MSRs have recently gained significant interest due to their potential for improved resource utilization, higher thermal efficiency, and passive safety characteristics. This summary focuses on liquid-fueled MSR designs. Early experimental research into MSR designs began with the Aircraft Reactor Experiment (ARE) [1], followed by the Molten Salt Reactor Experiment (MSRE) [2]. The Molten Salt Demonstration Reactor (MSDR) design was intended to scale up these experiments to demonstrate commercial viability [3]. Liquid-fueled MSR designs are more complex than traditional Light Water Reactors (LWRs) because they include flowing fuel salt that may be continuously processed and fueled during operation. This work leverages recent activities in developing modeling and simulation tools to address these complexities and operating modes.

This summary discusses preliminary studies of computational uncertainties for the Molten Salt Demonstration Reactor (MSDR) [3] using SCALE [insert SCALE reference here, at the first time SCALE is mentioned in the text and then renumber references as appropriate] sensitivity and uncertainty analysis tools and the SCALE/TRITON tool with continuous removal and feed capabilities. The uncertainty analyses herein provides a preliminary quantification of impacts for a reactor design's range of operational outcomes. Additional sensitivity analyses can help guide research directions, such as nuclear data or instrumentation development.

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UNCERTAINTY ANALYSIS WITH PARAMETER PERTURBATION

Using existing molten salt reactor neutronic and fuel cycle analysis tools within SCALE, a simple scoping analysis was performed on selected reactor parameters to understand the impact of uncertainties in these parameters on specific metrics using SCALE/SAMPLER [4].

The Molten Salt Demonstration Reactor Model

The MSDR is a graphite-moderated 750 MWt reactor designed to demonstrate commercial applicability of MSR technology. Assemblies in the core consist of rectangular graphite blocks between which fuel salt flows. A SCALE/TRITON [5] MSDR [3] quarter-assembly model (Fig. 1) was used to simulate a representative 3,500 days of MSR operation with continuous salt reprocessing.

The carrier salt is LiF with a lithium enrichment of 99.995% ^{7}Li . The fuel salt UF_4 is dissolved within the carrier salt to a high molar fraction (27.5%), with the uranium enriched to 4.95% specify wtNote that the MSDR design is not optimized (e.g., fuel-to-moderator ratio) for this fuel type. With a total salt volume of 41.3 m^3 and a salt density of 4.71 g/cm^3, the entire system contains 194.6 MT of fuel salt and 121.0 MT of heavy metal. For simplicity, the feed is selected to be constant in time at 0.85968 kg/day (9.95×10^{-3} g/s) of 4.95% ^{235}U low-enriched uranium (LEU).

A simplified set of separations are modeled: only noble gases and noble metals are removed, as the understanding is that these materials will tend to be released from the salt and may cause operational issues if not handled appropriately (Table I). Note that these effective half lives are very short and es-

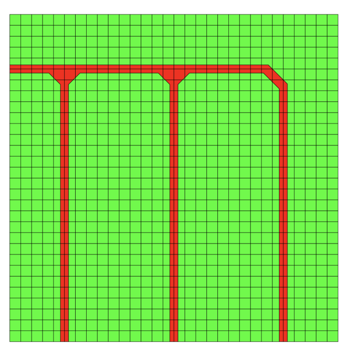

Fig. 1: Quarter of SCALE/NEWT model of the MSDR assembly cell showing fuel (red) and graphite (green).

TABLE I: Removal Rates and Materials for Depletion Simulations

Processing group	Elements	Effective $T_{1/2}$ (s)
Volatile gases	Xe, Kr, Ar, H, N, O	2.01
Noble metals	Se, Nb, Mo, Tc, Ru,	
	Rh, Pd, Ag, Sb, Te	2.01

sentially dominate the flow rate behavior; these materials are immediately removed from the system. Temperatures of the fuel salt and moderator are modeled as 898 K.

With the relatively low power density, thermal spectrum, and constant LEU feed rate, this converter reactor remains critical for 10 years.

Selection of Design Parameters and Responses

Parameters and their uncertainties were selected through a literature review [6], [7], [8], [3]. These selected parameters are not intended to be exhaustive, but are meant to demonstrate this analysis capability and identify the most impactful parameters (Table II). Uncertainties in these design parameters either represent physically known uncertainties or general unknowns (e.g., in processing system efficiency and design).

Several responses have been selected that span different applications and objectives (Table III). The isotopic inventories are quantified at End of cycle (EOC), with the exception of tritium, which is continuously removed from the salt and determined as the total generated tritium mass.

RESULTS

The responses from the unperturbed (nominal) simulation show that the neutron spectrum hardens over time (Fig. 2), and the assembly model maintains a critical configuration for 9.5 years (Fig. 3).

Two hundred realizations were generated for the perturbed configuration and the cases were run with SCALE/SAMPLER, with the selected uncertainties. The parameters were perturbed simultaneously(Table II). Three major parameters that have large correlations with responses are graphite density, power (burnup), and temperature (Figs. 4 and 5). The correlation values are calculated for each response-parameter value by the following equation:

$$\rho_{x,y} = \frac{\sum(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum(x_i - \bar{x})^2 \sum(y_i - \bar{y})^2}}$$

Since multiple parameters are perturbed for each simulation, the correlation values may not be as accurate as doing a sensitivity analysis for a single parameter. However, this approach

TABLE II: Parameters for the MSDR [3]

Parameter	Baseline	Uncertainty
Power [MW]	750	3%
Initial fuel salt Load [T]	121.02	0.5%
Graphite Density [g/cm^3]	1.7766	1.5%
Feed Rate [kg/day]	0.85968	0.15%
Feed Enrichment [%U235]	4.95	0.15%
Initial Enrichment [%U235]	4.95	1.5%
Gas Removal Rate [s^{-1}]	0.33	30%
Noble Metal Removal Rate [s^{-1}]	0.33	30%
Temperature [K]	898.15	6%
Decay after Depletion Step [days]	0.27	30%
^{7}Li Enrichment	0.99995	0.1%

TABLE III: Responses Selected to Span Different Applications and Objectives

Response	Unit	Description
k_{eff}	-	Reactor operation parameter
Pu isotopes	g	Plutonium isotope inventory
Odd A Pu:Total Pu	-	Plutonium quality
^{235}U	g	Fissile uranium isotope inventory
^{238}U	g	Fertile uranium isotope inventory
^{3}H	g	Total tritium generated
Total Pu	-	total plutonium inventory
^{244}Cm	g	Curium buildup inside the core

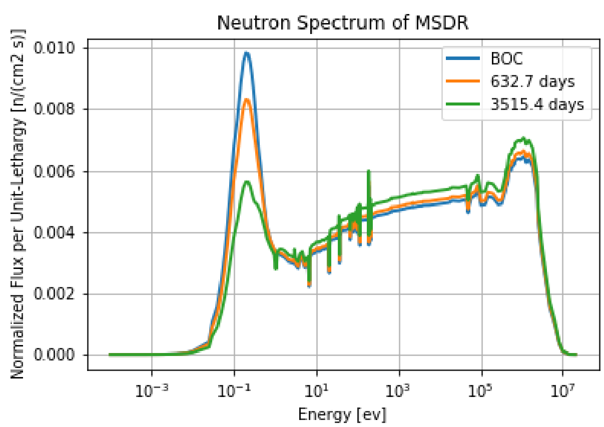

Fig. 2: Neutron spectrum of the MSDR cell model over time.

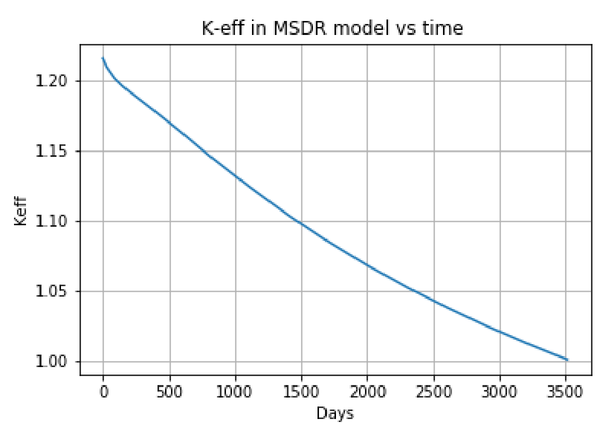

Fig. 3: The k_{eff} evolution of the MSDR cell model over time.

is a quick way to scope out impactful parameters.

Graphite density is positively correlated with criticality due to increased thermalization of neutrons and is negatively correlated with plutonium generation for the same reason. Higher burnups increase ^{244}Cm and ^{3}H generation, and decrease EOC ^{235}U inventory. The relationship between the three parameters and responses can be plotted as a scatter plot (Fig. 5), which provides more insight into the magnitude of the correlation between the parameter and response. Note that these trends are realized within an uncertainty analysis, meaning that more than one parameter is perturbed for each instance. Despite the high correlation between parameters and responses, the uncertainty of the parameters was small enough that most of the response uncertainty is less than 3% (Fig. 6), except ^{244}Cm .

DISCUSSION

Graphite density, power, and temperature are identified to have a substantial impact on MSDR operation. Other impactful parameters may be identified for different MSR designs (e.g., fast-spectrum MSRs will not contain graphite).

A further, more in-depth sensitivity study is planned for each identified important parameter. Future work also includes MSDR uncertainty analysis with SCALE/Sampler to assess the effect of uncertainties in nuclear data (e.g., cross sections, fission yield).

These sets of uncertainty analyses, along with sensitivity studies of identified parameters, provide insight into the instrumentation and monitoring improvements necessary to provide confidence in MSR modeling and simulation predictions and to ensure accurate operations of future MSRs.

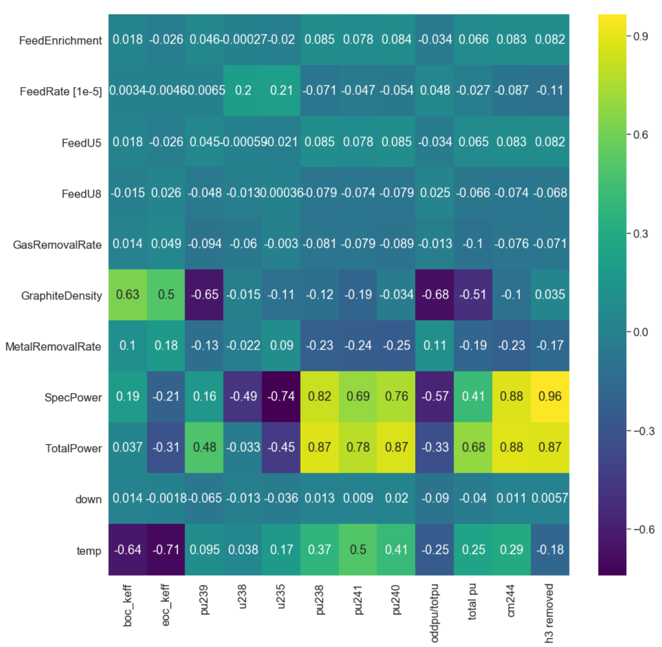

Fig. 4: Correlation heat map. Responses are listed in the x axis, and the parameters are listed in the y axis. This heat map provides insight into important parameters.

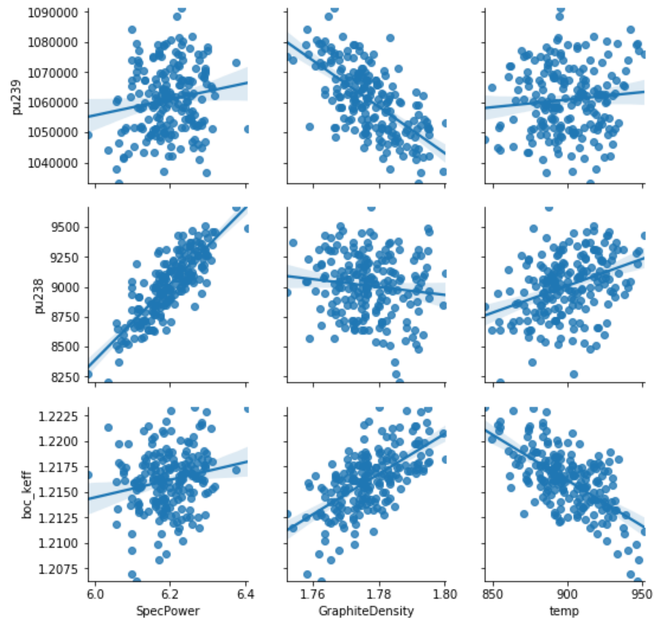

Fig. 5: Scatter plot and linear regression line for each major response–parameter set. Parameters are listed in the x axis, and responses are listed in the y axis.

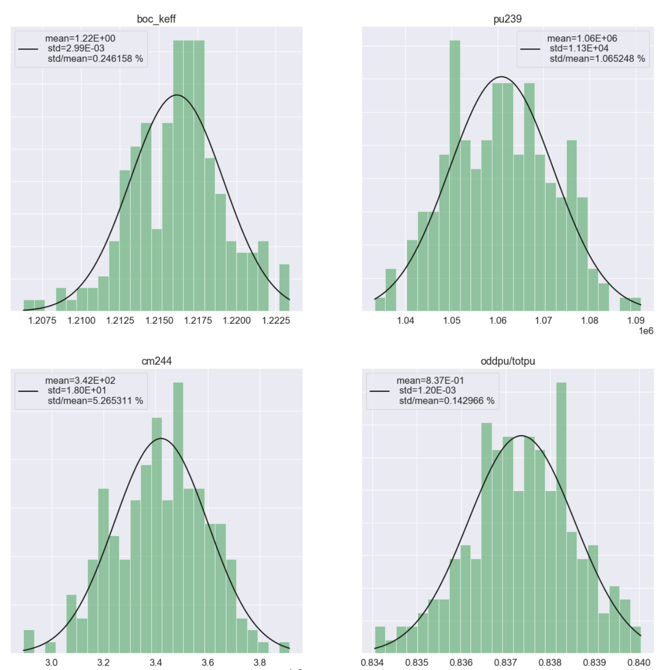

Fig. 6: Distribution of the response values (N=200). ^{244}Cm is the response with the largest uncertainty.

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